SPECTROSCOPY OF CHLOROSYL FLUORIDE, FCIO

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FCIO has been proposed as an intermediate in reactions involving CIF, Cl₂O, and CIF₃O, and it has been suggested as a molecule of atmospheric interest. It has been prepared in situ by the hydrolysis of CIF₃. The pure rotational spectrum of FCIO has been studied by conventional millimeter wave techniques and by microwave Fourier transform spectroscopy. Selected transitions were searched for using predictions based on an analysis of the ν_1 band.^a FCIO is an asymmetric prolate top, $\kappa = -0.8950$ for F³⁵CIO, with a rather small dipole component of 0.093 (4) D along the a-axis and a larger one of 1.93 (5) D along the b-axis. Transitions with $0 \le J \le 54$ and $0 \le K_a \le 18$ were observed. Cl hyperfine splitting was generally observable throughout the spectrum with ¹⁹F spin-rotation splitting observable as well in the microwave region. Structural parameters, harmonic force constants, and nuclear magnetic shielding parameters were derived and will be compared with data of related molecules, such as CIF₃, CIF, FCIO₂, and FCIO₃. High resolution infrared spectra were taken in the regions of the FCl stretching mode and bending mode around 600 and 310 cm⁻¹, respectively. A preliminary analysis indicates that the FCl stretch, near 596.86 cm⁻¹ for F³⁵ClO, is in resonance with the dark overtone of δ near 617 cm⁻¹. A brief progress report will be given.

Time required: 15 min

Session in which paper is recommended for presentation: 7

Comment: Please avoid conflicting sessions with the Miller & Cohen papers on IO and OIO and with contributions by G. Winnewisser

^aH. S. P. Müller, paper MF04, presented at The 53rd Ohio State University International Symposium on Molecular Spectroscopy, Columbus, OH, June 1998